Density matrix description of non-equilibrium quantum transport

PRASENJIT DUTT, JENS KOCH, CHUNG-HOU CHUNG, Department of Physics, Yale University, JONG HAN, Department of Physics, SUNY Buffalo, KARYN LE HUR, Department of Physics, Yale University — Interacting quantum systems and non-equilibrium phenomena both embody fundamental challenges in theoretical physics. Phenomena at the confluence of the two are in general not very well understood and suffer from a lack of a unifying theoretical description. In this work we focus on the nonlinear transport through a quantum dot maintained at a finite bias. Non-equilibrium quantum impurity models are reformulated in terms of the Lippmann-Schwinger operators which are used to construct a steady state density matrix and hence define an effective equilibrium. This facilitates the implementation of standard many-body techniques. We expand upon the work of Hershfield and show the equivalence of observables computed in the Keldysh approach and the density matrix formalism. We also show how to implement systematic perturbative as well as non-perturbative techniques using this scheme for the Anderson model far from equilibrium, in the limits of weak and large Coulomb interaction. This allows us to rigorously compute transport quantities such as the I-V characteristics and the spectral function, taking into account the full-bias dependence.